CANANOLAB 1.5

Installation Guide



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Introduction to caNanoLab

Welcome to the cancer Nanotechnology Laboratory (caNanoLab) 1.5 Installation Guide. caNanoLab is a data sharing portal designed to facilitate information sharing in the biomedical nanotechnology research community to expedite and validate the use of nanotechnology in biomedicine. caNanoLab allows researchers to share information on nanoparticles including the composition of the particle, the functions (e.g. therapeutic, targeting, diagnostic imaging) of the particle, the characterizations of the particle from physico-chemical (e.g. size, molecular weight, surface) and in vitro (e.g. cytotoxicity, blood contact) nanoparticle assays, and the protocols of these characterization.

As of release 1.1, the caNanoLab domain model has been caGrid enabled. In other words, a caNanoLab grid data service can be deployed and registered with caGrid production index server, allowing sharing of public nanoparticle information across the caGrid. In release 1.5, the caNanoLab grid service has been updated to use caGrid 1.3. For more information, see https://cabig.nci.nih.gov/workspaces/Architecture/caGrid.

Targeted Developer

The caNanoLab application development is best suited for an experienced Java developer who has some familiarity with the following J2EE and related technologies:



Important Background Knowledge

- Unix/Linux environment, Windows XP environment or Mac OS environment (Configuring environment variables; Installing Ant, JDK, Apache Tomcat and JBoss servers)
- Ant build scripts
- J2EE web application development using the Struts framework, Servlet/JSP's. JavaScript
- J2EE middle-ware technologies such as n-tier service-oriented architecture and software design patterns
- Hibernate Java persistence framwork
- caGrid 1.3 infrastructure (for understanding how a caNanoLab grid data service functions)

General System Requirements

The following open source technologies power a caNanoLab web application:

Open Source Technologies

- Java Software Development Kit (JDK) version 5.0
 http://java.sun.com/javase/downloads/index_jdk5.jsp
- JBoss version 4.0.5 http://labs.jboss.com/jbossas/downloads
- Jakarta Ant version 1.6.5 http://archive.apache.org/dist/ant/binaries/
- MySQL version 5.0.x http://dev.mysql.com/downloads/mysql/5.0.html

The caNanoLab web application has been tested within NCICB against JBoss servers (version 4.0.5) hosted on Windows XP and RedHat Linux systems, and against MySQL 5.0.45 databases hosted on RedHat Linux systems and MySQL 5.0.45 on Windows XP systems. Prior to release 1.2.1, the caNanoLab web application had been tested against Oracle 9i databases hosted on Sun Solaris systems, and Oracle 10g XE database hosted on Windows XP.

Download each of the tools listed in the bulleted list above and follow the installation instructions provided with each respective product for your environment. Assistance from a MySQL database administrator is expected to properly configure the MySQL database. For MySQL database configuration and maintenance, it is also helpful to download the MySQL 5.0 suite of GUI tools at http://dev.mysql.com/downloads/qui-tools/5.0.html.

Grid Service

Setting up a caNanoLab grid service is optional. It is recommended that you install the grid service only after you successfully install the web application and become familiar with submitting and searching data through the web application.

Grid Service Downloads

In release 1.5, there are no separate technology downloads required for installing the caNanoLab grid service, and most have been packaged within the caNanoLab source distribution file.

Obtaining the caNanoLab Source

Source Code

The caNanoLab web application source code and the caNanoLab grid service deployment war file are distributed as a zip file named caNanoLab_1.5.zip from the NCICB GForge site at http://gforge.nci.nih.gov/frs/?group_id=69_under_release_1.5

Database Technology

Assumptions and Requirements

The caNanoLab source distribution <code>caNanoLab_1.5.zip</code> has been downloaded from the NCICB GForge site. A MySQL database has been set up on a system (local or remote) with an administrator (or root) account. You should be familiar with the process of creating InnoDB tablespaces, databases creating users and assigning privileges to users.

For a Previous Installation

If you have installed caNanoLab prior to release 1.5 against an MySQL database, or release 1.2 or release 1.1.1 or release 1.1 against an Oracle database, and have associated production data in these schemas and you would like to continue to use the same data for caNanoLab release 1.5 in MySQL, review the following database initialization steps, then go directly to *Data Migration* on page 4. If you have a previously installed caNanoLab application running on a JBoss server, stop the server before running the database scripts.

For a New Installation

If you are installing the caNanoLab application for the first time or want to install a new schema for release 1.5, follow the steps below to set up the required MySQL schema objects and the seed data for release 1.5.

Initializing the MySQL Database

Follow these steps to initialize your MySQL database system:

Step	Action
1	Extract the cananolab_1.5.zip to a location on your local system, for example, C:\cananolab_1.5. This location is referred as <cananolab_source> throughout the document. Verify that the following seven SQL scripts exist in the directory <cananolab_source>/db/1.5:</cananolab_source></cananolab_source>
	• mysql_seed.sql
	• create_database_and_user.sql
	• app_schema.sql
	• insert_common_lookup.sql
	• csm_schema.sql
	• csm_priming_data.sql
	• app_csm_priming_data.sql
	Note: The scripts <code>create_database_and_user.sql</code> create a new 1.5 schema canano and a new database user cananolab_app with required privileges and a password go!234. If you'd like to create a different database user, be sure to modify this script and make a note of the information for later use

Step	Action
	in setting up the caNanoLab application.
	User administration and schema privileges can also be managed by the MySQL Administrator GUI as a part of the MySQL 5.0 suite of GUI tools.
2	Log into the MySQL database as the database administrator (root) and go to the directory <cananolab_source>/db/1.5 and execute the script mysql_seed.sql to set up a schema named canano and its required seed data.</cananolab_source>
	Example: On a Windows XP system hosting a MySQL 5.0.45 database, you would issue the following commands at the DOS prompt (assuming the root account has password rootpass):
	C:\>cd C:\caNanoLab_1.5\db\1.5
	<pre>C:\caNanoLab_1.5\db\1.5\>mysql -h localhost -u root - prootpass <mysql_seed.sql< pre=""></mysql_seed.sql<></pre>

Verification

Once the MySQL database has been created, either through new setup or through data migration (described in the next section), verify that the following numbers of database objects are created:

• Tables 66

Example: Issue the following query at the MySQL prompt, logging in as cananolab app:

```
mysql> select count(*) from information_schema.tables
where table_schema='canano' and table type='BASE TABLE';
```

Data Migration

NOTE:



If you are installing caNanoLab 1.5 for the first time or installing a new caNanoLab release 1.5 schema, you can skip this section.

This installation guide only discusses the steps for migrating from release 1.4.1.2 in MySQL to release 1.5 in MySQL. If you have previously installed caNanoLab in MySQL prior to release 1.4.1.2, you'd have to migrate to release 1.4.1.2 first, one release at a time. Please see the install instructions for each release at http://gforge.nci.nih.gov/frs/?group_id=69 for details.

Follow these steps to complete the required data migration from release 1.4.1.2 in MySQL to release 1.5 in MySQL:

Step	Action
1	Extract the cananolab_1.5.zip to a location on your local system, for example, C:\cananolab_1.5. This location is referred as <cananolab_source> throughout the document. Verify that the following SQL scripts exists in the directory <cananolab_source>/db/1.5:</cananolab_source></cananolab_source>
	• insert_common_lookup.sql
	<pre>and the following ten SQL scripts exist in <cananolab_source>/db/1.5/data_migration:</cananolab_source></pre>
	• migration_general.sql
	• common_lookup_migration.sql
	• sample.sql
	• nanomaterial_entity.sql
	• poc_migration.sql
	• instrument_migration.sql
	• datum_migration.sql
	• characterization_migration.sql
	• csm_migration.sql
	• migration_to_csm_4.1.sql
	Note : If you institute has data that we haven't accounted for in the automated data migration scripts, please notify the caNanoLab technical team. Specialized migration scripts may be necessary.
2	Log into the MySQL database as the database administrator (root) and go to the directory <cananolab_source>/db/1.5/data_migration and execute the following script in the order specified:</cananolab_source>
	• migration_general.sql
	Example: On a Windows XP system hosting a MySQL 5.0.45 database, you would issue the following commands at the DOS prompt (assuming the root account has password rootpass):
	C:\>cd C:\caNanoLab_1.5\db\1.5\data_migration C:\caNanoLab_1.5\db\1.5\data_migration>mysql -h localhost -u root -prootpass <migration_general.sql< td=""></migration_general.sql<>
	Note : If you have a lot of data in the database, the script may take several minutes to complete. Don't quit the execution until it's done.

After data migration, refer to the Verification section on page 4 to verify that the migration has been successful. There will be 67 instead of 66 schema objects. The extra table <code>instrument_to_review</code> contains instruments that are not automatically migrated and requires manual review.

caNanoLab Web Application

Assumptions and Requirements

The database has been installed and verified, as described on pages 3 through 5. Ant has been installed. The JBoss application server has been installed on a system (local or remote) and can be started at a designated port. JBoss install directory is referred as <JBOSS_HOME> in the document. The JBoss application server host URL is referred as <APP_SERVER_URL>, for example, cananolab-dev.nci.nih.gov:19080. It is assumed that the default configuration is used for deploying caNanoLab web archive files. For example, in JBoss 4.0.5, the default configuration is located at the directory <JBOSS_HOME>/server/default. The caNanoLab web archive file shall be deployed at the directory <JBOSS_HOME>server/default/deploy.

It is possible to configure Apache server to interface with the JBoss server and set up a virtual host for the caNanoLab application, if you need assistance, please contact NCICB Application Support (info provided at the end).

Installation and Deployment

Follow these steps to install and deploy caNanoLab.

Step	Action
1	Set up an environment variable JBOSS_HOME to point to the JBoss installation directory.
	Note: Either double back slashes \\ or a single forward slash / should be used as the file separator if working on Windows platform, for example, \\ JBOSS_HOME=C:/jboss-4.0.5.GA (C:\jboss-4.0.5.GA would fail).
2	Edit the Ant build properties file build.properties at <cananolab_source> by specifying values for the following three properties:</cananolab_source>
	 a. file.repository.dir: a directory on the system that hosts the JBoss application server for storing uploaded files, for example, C:/caNanoLab/fileupload.
	Note: This directory should be writable by the user that starts the JBoss server, and this directory should be created prior to starting the application. Either double back slashes \\ or a single forward slash / should be used as the file separator if working on Windows platform.
	b. application.owner: the owner of the caNanoLab release 1.5 installation

Step	Action
	instance, for example, NCL. grid.indexserver: the grid index server from which the caNanoLab grid data services can be automatically discovered, for example, http://cagrid-index.nci.nih.gov/:8080/wsrf/services/DefaultIndexService , the NCICB's production caGrid index server.
3	Edit the Ant build properties file deploy.properties at <cananolab_source> by specifying values for the following four properties: a. database.host: the host name of the server hosting the database, for example, localhost b. database.port: the database port number, for example, 3306 c. database.user: the database user name used in the caNanoLab application, for example, cananolab_app. Please refer to page 3. d. database.password: the password for the database user specified above, for example, go!234</cananolab_source>
4	Execute the Ant build script build.xml located at <cananolab_source> with the target deploy-application. Example: Issue the following commands to execute the Ant script: C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant deploy-application Successful execution of the Ant script creates two deployable web archive war files in the directory <cananolab_source>/build: caNanoLab.war and upt.war, and places these two wars to the JBoss deploy directory, for example, <jboss_home>/server/default/deploy.</jboss_home></cananolab_source></cananolab_source>
5	Execute the Ant build script build.xml located at <cananolab_source> with the target prepare-csm-conf. Example: Issue the following commands to execute the Ant script: C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant prepare-csm-conf Successful execution of the Ant script sets up the required CSM 4.1 configurations in the JBoss server. The caNanoLab web application relies on a modified version of NCICB CSM (Common Security Module) version 4.1 for user authentication and role-based authorization. For more information, see the CSM documentation at http://gforge.nci.nih.gov/frs/?group_id=12. Note: Since we've migrated CSM from version 3.1 to version 4.1, the required configuration for the JBoss server has changed. You should not skip this step.</cananolab_source>

Step	Action
6	Execute the Ant build script build.xml located at <cananolab_source> with the target reset-csm-db-connection.</cananolab_source>
	Example: Issue the following commands to execute the Ant script:
	C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant reset-csm-db-connection
	Successful execution of the Ant script sets up the required CSM 4.1 configurations in the database.
7	Execute the Ant build script build.xml located at <cananolab_source> with the target reset-passwords.</cananolab_source>
	Example: Issue the following commands to execute the Ant script:
	<pre>C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant reset-passwords</pre>
	Successful execution of the Ant script resets all user passwords to be their logins. This is necessary as the password encryption scheme used in CSM 3.1 and 4.1 are not the same.
	Note : After caNanoLab 1.5 is installed, when a user logs in the caNanoLab application for the first time, he/she will be prompted to change password.
8	Execute the Ant build script build.xml located at <cananolab_source> with the target set-sample-associated-visibility with two arguments curator.login.name and curator.password, where curator.login.name is the login name for the user account that has been assigned the curator role, and curator.password is the password for the curator account.</cananolab_source>
	Example: Issue the following commands to execute the Ant script:
	<pre>C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant set-sample-associated-visibility - Dcurator.login.name=janedoe -Dcurator.password=janedoe</pre>
	Successful execution of the Ant script sets up required access privileges for all data associated with samples.
	Note : After step 7, the curator password has been initialized to be the same as the curator login. The old password no longer works.
	If there are many samples in the schema, this step may take sometime to complete. Please be sure to wait until completion of the execution.

Step	Action
9	When deploying both the caNanoLab application and the caNanoLab grid service (see page 12)to the same JBoss server, we recommend increasing the JBoss JVM heap size to 1G bytes and permanent generation (permgen) memory space to 512M bytes by updating the file <jboss_home>/bin/run.conf with the following JAVA_OPTS: JAVA_OPTS="-Xms512m -Xmx1024m -XX:PermSize=256m - XX:MaxPermSize=512m -Dsun.rmi.dgc.client.gcInterval=3600000 -Dsun.rmi.dgc.server.gcInterval=3600000" This configuration file is read when JBoss server starts.</jboss_home>
10	When deploying the caNanolab application and the grid service in a production environment, we also recommend updating the default logging behavior of the JBoss server by turning off the unnecessary loggings thus reducing file system requirements for server log files. Please locate the file <jboss_home>/server/default/conf/log4j.xml and add to the beginning of the section Limit categories the following text: <!-- ===================================</td--></jboss_home>
	<pre></pre>

Step	Action
	<pre><category name="CSM"></category></pre>
	-end of edit for caNanoLab

Verification

Once the deployment war files have been deployed and the JBoss application server is correctly configured, you can now start the JBoss application server, which in turn starts the caNanoLab application.

Open the URL http://cananolab/ (for example, http://cananolab-dev.nci.nih.gov:19080/caNanoLab). You should see a disclaimer page. Click on **CLICKING HERE** to go to the Welcome/Login page.

User Provisioning Tool (UPT)



Creating User Accounts

Before users can log in to the caNanoLab application to submit and search data, you must first create their user accounts and assign them to the predefined user groups with the pre-defined roles to access the pre-defined protection groups. The caNanoLab application makes use of the NCICB's User Provisioning Tool (UPT), a separate web application, for user account management. The concepts of users, groups, roles, protection groups are defined according the CSM/UPT principles. See the CSM documentation at http://gforge.nci.nih.gov/frs/?group_id=12 for details on these concepts and the use of the UPT tool.

In release 1.5, as a part of the database seed data, a default user group Public has been created and has been assigned role R to protection group protocol, sample and publication, i.e. assigned access to search public protocols, samples and publications.

During the caNanoLab application start up, two more default users groups are auto-generated: <application.owner>_Curator, <application.owner>_Researcher, where the value for <application.owner> is specified in the file build.properties prior to building the application as described on page 6. At start up, <application.owner>_Curator is assigned role CURD to protection group protocol, sample, and publication, i.e. assigned access to submit and update protocols, samples and publications.

When a user in the <application.owner>_Curator group submits data (protocols, samples, publications) into the caNanoLab system, the data is automatically assigned to be visible for the two default groups.

NOTE:



In release 1.5, a user must be assigned as a caNanoLab administrator to see the ADMINISTRATION menu item in the application to log into the UPT tool or do update site preferences such as site logo.

UPT Example

The following steps illustrate an example use of the UPT tool to create a new user, to assign the user to be a caNanoLab administrator, and to assign the user to a pre-defined user group.

Step	Action
1	Launch the UPT tool at <a href="http://<APP_SERVER_URL>/upt">http://<app_server_url>/upt</app_server_url> and login as superadmin/superadmin . Use csmupt as the application name when prompted at the UPT log in.
	Note: The user superadmin with initial password superadmin was created as a part of the database setup. Only superadmin can assign users to be caNanoLab administrators.
2	Once logged into the UPT tool, follow these steps to reset the password for <i>superadmin</i> :
	 a. Select User > Select an Existing User. b. Click on Search and select superadmin and click on View Details. c. Update the User Password field and Confirm Password field and click on Update to commit the change.
3	Logged in as the super admin, follow these steps to create a new user: d. Select User > Create a New User . e. Create a new user account named admin with an initial password.
	 f. Select Application > Select an Existing Application; click Search. g. Select caNanoLab from the application list. h. Click View Details, then Associated Admins.
	 i. Assign this user to be an administrator for the caNanoLab application. j. Click Update Association to commit the change.
4	Log out of the UPT tool and log back in as admin . Use caNanoLab as the application name when prompted at the UPT log in.

Step	Action
5	Select User > Select an Existing User, and click Search. Select admin from the User list. a. Click View Details, then Associated Groups. b. Select <application.owner>_Curator from the pre-defined group list and assign it to the user. c. Click Update Associations to commit the change.</application.owner>

Follow similar steps to create other application user accounts and to assign them to different users groups, as appropriate.

NOTES:	 In release 1.5, superadmin or caNanoLab administrators assign the initial password when creating a new user account. The UPT tool doesn't allow users to manage their own passwords. Users can only update their passwords within the caNanoLab application by clicking on the Update Password link on the home page. Only users assigned as caNanoLab administrators and assigned to the <application.owner>_Curator group can delete information from caNanoLab.</application.owner> Publicly available data can be browsed through Browse caNanoLab links on the home page without logins. Users logged into the application have to be assigned to one of the predefined user groups to be able access protected data. A user can be assigned to multiple user groups. Roles and protection groups are assigned only to user groups, not users. During sample creation, the organization name of the primary point of contact associated with the sample is automatically created as a new user group, and the new sample is automatically assigned role R to the powdy greated user groups.
	contact associated with the sample is automatically created as a new

For more information about how to use the UPT tool for managing user accounts, contact NCICB Application Support at nci.nih.gov and request that the caNanoLab technical team give you a demonstration of the UPT tool in the context of the caNanoLab application.

caNanoLab Grid Data Service

Assumptions and Requirements

The JBoss server has been downloaded, installed and configured correctly, and the release 1.5 caNanoLab application has been correctly installed. If you had started the JBoss server to test the caNanoLab application installation, please shut it down now. In release 1.5, the caNanoLab grid service is configured to be deployed to the Tomcat embedded in the same JBoss server used for deploying the caNanoLab application. Users are no longer required to install a separate Tomcat server or to download and install Globus Toolkit.

In order for the grid service to successfully register with the NCICB production index server, the server and the port number hosting the JBoss server must be publicly accessible.

Installation and Deployment

Follow these steps to create and deploy a caNanoLab grid data service.

Step	Action
1	If not done already, set up an environment variable <code>JBOSS_HOME</code> to point to the <code>JBoss server</code> install directory as in step 1 on page 6.
	If not done already, edit the Ant build properties file build.properties at <cananolab_source> as in step 2 on page 6.</cananolab_source>
	If not done already, edit the Ant build properties file deploy.properties at <cananolab_source> as in step 3 on page 7.</cananolab_source>
	Note : the value of the property application.owner is used to construct the site name shown in the Site drop-down list on the caNanoLab home page.

Step	Action
2	Edit the Ant build properties file <code>grid.properties</code> at <cananolab_source> by specifying values for the following properties:</cananolab_source>
	 a. grid.service.hostname: virtual host name for the server hosting JBoss, for example, cananolab-dev.nci.gov b. grid.service.port: port number configured for the Tomcat service embedded in JBoss, for example, 19080 c. country: the country in which the caNanoLab grid service is running, for example, US. d. city: the city at which the caNanoLab grid service is running, for example, Rockville. e. zipcode: the zip code at which the caNanoLab grid service is running, for example, 20852. f. state: the state at which the caNanoLab grid service is running, for example, MD. g. street1: the first part of the street at which the caNanoLab grid service is running, for example, 2115 East Jefferson Street. h. street2: the second part of the street at which the caNanoLab grid service is running. i. affiliation: the affiliation of the person who is responsible for maintaining the caNanoLab grid service, for example, NCICB. j. email: the email of the person who is responsible for maintaining the caNanoLab grid service, for example, ncicb@po.nih.gov k. phone: the phone number of the person who is responsible for maintaining the caNanoLab grid service. l. first.name: the first name of the person who is responsible for maintaining the caNanoLab grid service. m. last.name: the last name of the person who is responsible for maintaining the caNanoLab grid service. Note: Properties c through g are grid service metadata that are required for the grid index server to visually map the location of a grid service in the caGrid portal, and are useful during grid service auto-discovery. Properties h through m are optional, but useful information for others to look up the grid service.
3	Execute the Ant build file build.xml located at <cananolab_source> with the target deploy-grid. For example, C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant deploy-grid</cananolab_source>
	Successful execution of the Ant build script generates a war file wsrf-canano.war at the <cananolab_grid_source>/build directory and places the war file to the JBoss deploy directory, for example, <jboss_home>/server/default/deploy.</jboss_home></cananolab_grid_source>

Step	Action
4	Execute the Ant build script build.xml located at <cananolab_source> with the target prepare-globus-lib. For example,</cananolab_source>
	C:\>cd C:\caNanoLab_1.5 C:\caNanoLab_1.5>ant prepare-globus-lib
	Successful execution of the Ant build script extracts eight jar files for deploying Globus to the JBoss server at <jboss_home>/server/default/lib.</jboss_home>
5	If not done already, follow step 9 and 10 on pages 9 and 10 to configure appropriate memory and logging settings for the JBoss server.

Verification

Once the grid service war file has been deployed and you have correctly configured JBoss server with required Globus libraries, you can now start the JBoss server, which in turn starts the caNanoLab application and the caNanoLab grid service. To verify the creation of the caNanoLab grid data service, open the URL http://cananoLabService, for example, http://cananolab-dev.nci.nih.gov:19080/wsrf-canano/services/cagrid/CaNanoLabService. You should see a page that says:

cagrid/CaNanoLabService

Hi there, this is an AXIS service!

It takes more than ten minutes for the grid service to successfully register in the index server. Wait some time and go into the caGrid portal at http://cagrid-portal.nci.nih.gov/web/guest/home. You should see your grid service showing up on the portal map. This completes the release 1.5 installation.

Note: After successful registration with the production grid index server, your grid service name will show up as a remote site in the **Site** drop-down list on the home pages of other caNanoLab deployments.

For more information and help on caGrid service configuration and deployment, refer to the caGrid wiki page: http://www.cagrid.org.

If you need further assistance on setting a caNanoLab grid service, contact NCICBIT Application Support at nci.nih.gov and request that the caNanoLab technical team help you with caNanoLab grid service.

Contacting Application Support

NCICB Application Support http://ncicb.nci.nih.gov/NCICB/support ncicb@pop.nci.nih.gov

Telephone: 301-451-4384 Toll free: 888-478-4423